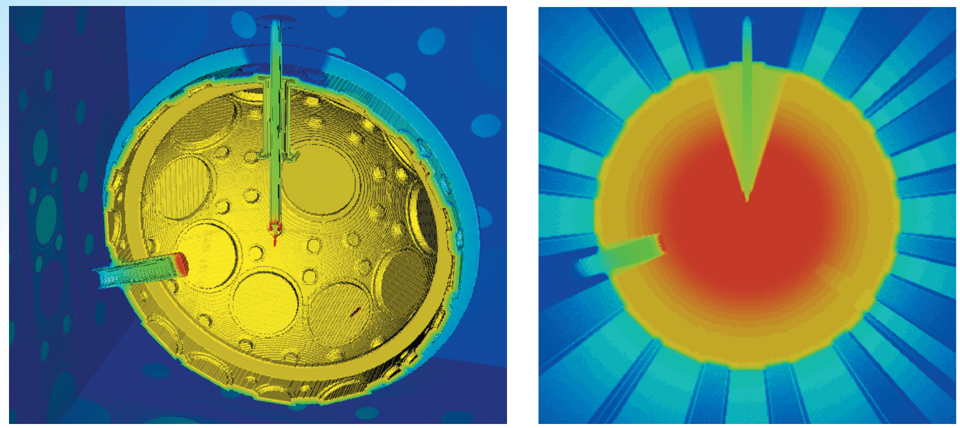
ITS

Institute for Terascale Simulation

Center for Applied Scientific Computing



Total neutron scalar flux values are shown at the center plane of the Nova target chamber (ARDRA)

ASCI Institutes at the national defense laboratories collaborate with academia on research topics in computer science, computational mathematics, and scientific computing that are relevant to the Stockpile Stewardship Program (SSP). Each project focuses on an identified need of the ASCI code groups and corresponds to a technical area of importance. A CASC permanent staff member and at least one university collaborator lead each technical area. Current areas and researchers are described in the following paragraphs.

Scalable Linear Solver

Robert Falgout, CASC, and Steve McCormick, University of Colorado

This project develops scalable algorithms and software for the solution of large, sparse linear systems of equations on massively parallel computers. The project conducts algorithm research in three main areas:

- Geometric multigrid methods for structured mesh problems.
- Algebraic multigrid methods for unstructured mesh problems.
- Sparse approximate inverse and incomplete factorization methods as more general-purpose matrix solvers for structured, unstructured, and nonsymmetric problems.

Nonlinear Differential Equations

Carol S. Woodward, CASC, and David Keyes, Old Dominion University

This project investigates solution strategies for large-scale, time-dependent systems arising from the discretization of coupled, nonlinear, multiphysics models. Investigations have focused on the following areas:

- Nonlinear solvers, such as Newton—Krylov methods preconditioned with multigrid and nonlinear multigrid techniques, for both algebraic and PDE-originated nonlinear systems.
- Nonlinear preconditioners of Schwarz type.
- Time step selection methods, including BDF stability regions and semi-implicit schemes.
- Methods for analyzing the sensitivity of solution components to model parameters for systems of nonlinear equations, ODEs, and DAEs.

These methods have been applied to coupled radiation diffusion with material energy transfer, as well as to variably saturated porous media problems.

Transport Methods

Peter Brown, CASC, and Thomas A. Manteuffel, University of Colorado at Boulder

This effort develops scalable algorithms for the time-dependent and steady-state equations that model the flow of neutral particles through materials. The emphasis is on the development and implementation of methods for the parallel solution of the Boltzman transport equation, as well as radiation transport modeled by diffusion. Research considers the use of multilevel solution strategies in traditional solution approaches, as well as pursuing the development of new ones. First-Order Systems of Least Squares (FOSLS) methods show great potential for providing more accurate and robust solution procedures than traditional discrete ordinates approaches.

Adaptive Mesh Refinement

Rich Hornung, CASC, and Alejandro Garcia, San Jose State University

This project researches parallel adaptive mesh refinement (AMR) methods for a variety of multiphysics applications. AMR provides both spatial and temporal mesh refinement to focus computational resources where they are needed most in a computational domain. Problems under study include hybrid continuum-particle approaches for gas dynamics interface instabilities, laser-plasma instabilities, and hybrid adaptive ALE methods for shock hydrodynamics. Each of these simulation efforts emphasizes coupled physics models, advanced numerical methods, and dynamic mesh data structures. These research projects will guide the development of local refinement capabilities in future ASCI application codes.

Memory System Performance

Bronis R. de Supinski, CASC, and Sally A. McKee, University of Utah

The time to access main memory dominates the performance of large memory codes typically used at LLNL. This fact leads to poor CPU utilization because main memory accesses are orders of magnitude slower than CPUs.

Worse, Moore's law indicates that the memory wall problem will increase over time. Dynamic access ordering (DAO) mechanisms are techniques that change the order of memory accesses from that generated by the issuing program. They have been shown to have great promise to alleviate the problem of access time. Previously, researchers have focused on DAO techniques for uniprocessor systems; our project is extending DAO mechanisms to multiprocessor access issues, such as cache coherency and fairness, that do not arise in uniprocessor systems.

Software Technologies

Scott Kohn, CASC, and Dennis Gannon, Indiana University

The goal of this project is to improve both the development process and the performance of large-scale scientific applications by investigating and developing new software technologies and tools. There are three primary areas of research and development:

- The Component Technology effort is investigating the application of software component technology to scientific applications in a high-performance, massively parallel environment.
- The Parallel Performance Improvement effort is investigating parallel programming models and the associated tools to improve the efficiency of parallel code.
- The MemWall project is investigating techniques for examining and rearranging memory access requests in application codes to improve cache utilization.

Data Exploration

Sam Uselton, CASC, Charles Hansen, University of Utah, and Bernd Hamann, University of California at Davis

This project develops tools that enable more effective use of the data generated by applications running on the ASCI platforms. This project conducts research and development in four main areas:

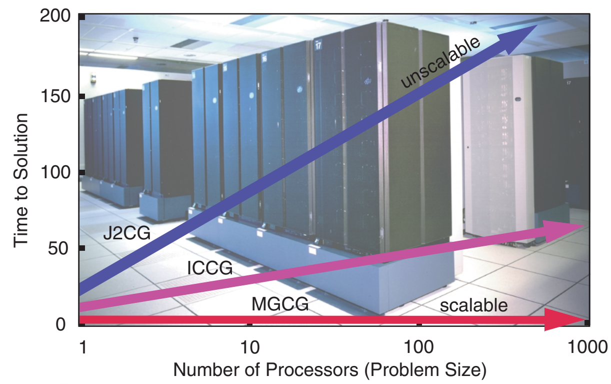
- Data management.
- Data discovery.
- Scientific visualization.
- User interfaces and displays.

Academic Collaborations

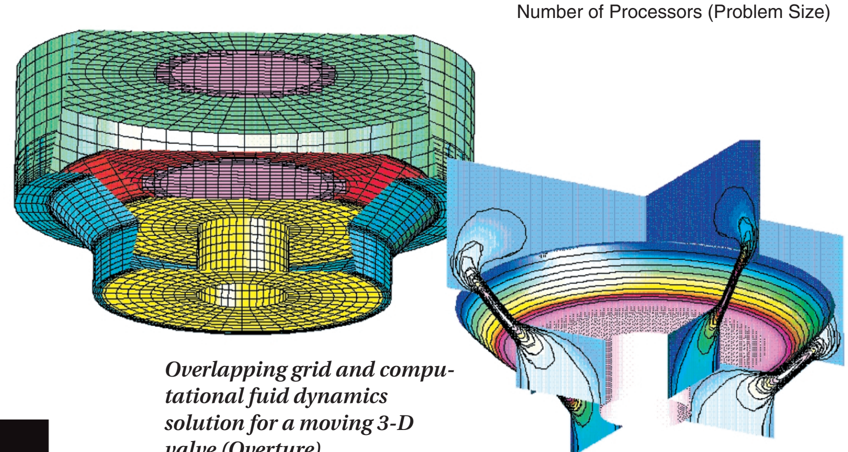
Steve F. Ashby, CASC, and David Keyes, Old Dominion University

The Institute encourages additional academic collaborations via the following:

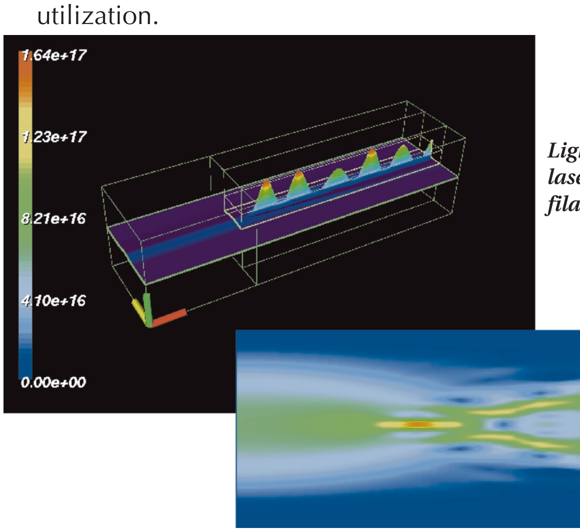
- ITS Postdoctoral Fellowships.
- Sabbatical Visitor Program focusing on particular needs.
- Summer Visitor Program for short-term research collaborations.
- Workshops to focus attention on particular techniques or applications critical to the SSP mission.
- Short courses to provide brief intensive periods of training in new techniques and technologies.



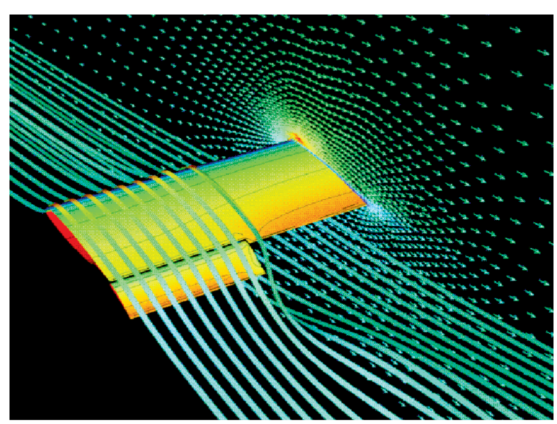
Scalable linear solvers (such as multigrid-preconditioned Krylov methods) enable terascale simulation



Overlapping grid and computational fuid dynamics solution for a moving 3-D valve (Overture)



Light intensity from a laser– plasma simulation of filamentation (SAMRAI)



Unstructured Mesh CFD Application

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